Semiclassical Molecular Dynamics: a useful Tool for Spectroscopic Interpretation

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I will present some novel theoretical methods based on semiclassical molecular dynamics and designed for spectroscopy calculations (for example IR) of high dimensional and/or condensed phase systems. These approaches are predictive. They are either based on a "divide-and-conquer" strategy, whereby the full dimensional spectra are obtained as a composition of several lower dimensional ones, or they exploit hierarchically the different levels of accuracy of different semiclassical propagators.[1-5] All methods provide frequency estimates whose Mean Absolute Error is generally within 10-20 wavenumbers of exact quantum mechanical results (when available), or experiments. The methods can be interfaced easily to ab initio molecular dynamics simulations allowing one to treat pretty large systems.[6-9] I will illustrate some applications involving several gas phase and some condensed phase systems.

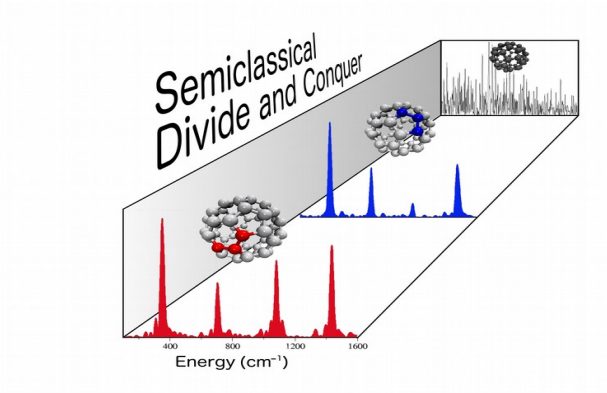

Figure: Spectroscopic representation of the "Divide-and-Conquer" Semiclassical Molecular Dynamics

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